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FRAGMENTS FROM DISSOC. (U) ARIZONA UNIV TUCSON OPTICAL
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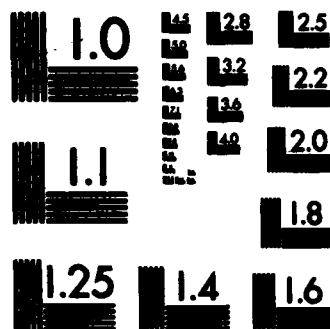
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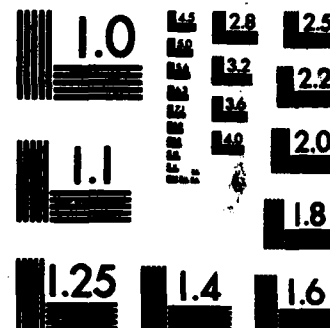


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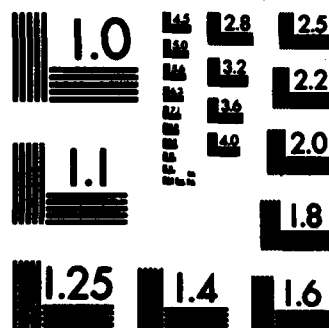
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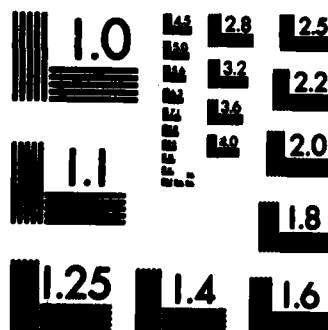
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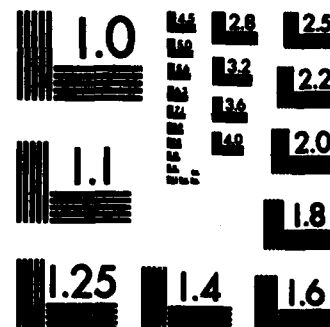
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20. ABSTRACT (Continue on reverse side if necessary and identify by block number) Progress is reported on research in molecular physics involving electron-bombardment molecular dissociation. The velocity distribution of metastable and ionic fragments are measured using a pulsed electron beam and a time-of-flight technique. During the past year, experiments involving detection of ionic fragments from the hydrogen halides and acetylene have been underway. The velocity spectrum of protons resulting from dissociation of the hydrogen halides show several distinct features, and attempts are presently being made.		

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to assign these features to particular molecular states. Measurements to determine electron bombardment threshold energies for these features have been made and should help in confirming such assignments. Several different ionic fragments have been detected from the dissociation of acetylene. A mass filter is used in these experiments to obtain velocity spectra of each mass species separately.

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Annual Technical Report
"Time-of-Flight Spectroscopy of
Ionic and Metastable Fragments from Dissociating Molecules"

Principal Investigators

Willis E. Lamb, Jr., Professor of Physics and Optical Sciences

K. C. Hsieh, Associate Professor of Physics

L. C. McIntyre, Jr., Professor of Physics

AFOSR Grant 80-0218

Summary of research June 1981 - June 1982

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Department of Physics and Optical Sciences Center

University of Arizona

Tucson, Arizona 85721

September 8, 1982

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I. Research Status

A. Introduction

This report contains a summary of research in molecular physics conducted under AFOSR grant 80-0218 during the period 15 June 1981 to 14 June 1982. The research was done in the Department of Physics at the University of Arizona by faculty and staff of the Department of Physics and Optical Sciences Center. The major objectives stated in our proposal for this contract period were:

1. Study the hydrogen fragments from dissociation of the hydrogen halides.
2. Study the dissociation fragments from H_2O and H_2S .
3. Investigate mass-resolved ionic fragments from light hydrocarbons.
4. Coincidence detection of fragments from H_2 dissociation.

The major effort during the past year has been directed toward items 1 and 3, although some work was done on the other two items. Several major advances in our experimental techniques were made during the past year. These include the addition of a digital-to-analog (DAC) converter to our computer-controlled data acquisition system. The DAC, when used in conjunction with programmable power supplies, allows us to change electron bombardment energy by computer control. This allows rapid sequencing of bombarding energies and greatly improves threshold measurements by averaging over any drifts in experimental conditions. Another improvement involved computer control of an arbitrary waveform generator used to provide the time-dependent potential barrier used in our ion mass filter.¹

Our experiments consist of time-of-flight measurements of metastable and ionic fragments resulting from electron bombardment dissociation of molecules. The electron beam is pulsed and intersects a beam of molecules, some of which dissociate producing fragments with a few eV kinetic energy. The fragments traverse a path of approximately 20 cm in a direction perpendicular to both the electron and molecular beams and are then detected. A velocity spectrum is accumulated by measuring the

distribution of time intervals between an electron beam pulse and a fragment detection. In some cases, information on repulsive states of the excited molecule can be inferred from the velocity distribution of the fragments. Details of specific experiments are given in the following paragraphs.

B. Dissociation fragments from the hydrogen halides

The kinetic energy spectrum of H^+ fragments from HCl at electron bombarding energies above about 30 eV has several distinct features. Spectra at 50 and 100 eV electron energies are shown in Fig. 1. Prominent peaks occur at approximately 7.5, 5.5, and 4.5 eV; and there are several additional features below 3 eV. In our attempt to identify the repulsive molecular states responsible for these peaks, the measurement of appearance thresholds has proved very useful. The threshold electron bombardment energy is used to locate the position of the repulsive potential in the Franck-Condon region. The observed kinetic energy of the fragments is then subtracted from this threshold to locate the energy of the separated atom asymptote. In this manner, we can limit the number of possible repulsive states which could be responsible for a particular feature to those corresponding to a particular separated atom limit.

Recent results on the 7.5 eV feature give a threshold at about 22 eV which implies that the repulsive state asymptote is located at about 14.5 eV. This corresponds to a separated atom limit of $H^+ + Cl^-$. Our initial guess that this feature was the result of dissociation of the $B^2\pi$ state which dissociates into $H^+ + Cl(g.s.)$ was proved wrong by the threshold measurement. The other two high energy peaks at 5.5 and 4.5 eV are found to result from states with separated atom limits of 31.5 and 23.5 eV, respectively. Work is continuing on HCl as well as HF, HBr, and HI.

C. Mass resolved ionic fragments from light hydrocarbons

Our recent experiments on H^+ , H_2^+ , and H_3^+ fragments from electron-bombardment-dissociated methane, ethane, methanol, and ethanol have demonstrated the usefulness of mass-resolved ion velocity measurements.² A knowledge of the ion's

mass allows a direct determination of its kinetic energy distribution. We have started an investigation of ionic fragments from acetylene (C_2H_2) using our improved mass filter which has a computer-controlled arbitrary waveform generator to produce the time-dependent potential barrier.

Our initial mass scans have produced kinetic energy distributions of H^+ , C^+ , CH^+ , and CH_2^+ fragments. These first preliminary results are shown in Fig. 2. We plan to extend this work to several electron bombarding energies and to search for H_2^+ and C_2H^+ fragments. We also plan to extend these measurements to other light molecules such as C_2H_2 , C_6H_6 , and NH_3 .

D. Other experiments

We have two additional projects in various stages of completion. Some work was done during the past year on detecting H^+ fragments from dissociation of H_2O . Between 60 and 100 eV electron bombarding energy, the principal feature in the H^+ kinetic energy spectrum is a broad peak centered at about 1.5 eV which extends to approximately 7 eV where the intensity is about 1/10 the peak intensity. At energies near 100 eV a possible additional feature at about 7 eV is seen to appear. Additional work on H_2O including threshold measurements and extension to H_2S is planned for the near future.

Another experiment on which progress was made during the past year was the attempt to detect H^+ and $H(2s)$ fragments from dissociation of H_2 . There are two known excited states of H_2^+ that dissociate into $H^+ + H(2s)$ fragments and we plan to detect these oppositely moving fragments in coincidence. The equipment for this experiment has been assembled and is presently installed in our vacuum chamber. Preliminary tests have been made on the electronics required to detect coincidences and we hope to begin running soon on this experiment.

References

1. M. D. Burrows, S. R. Ryan, W. E. Lamb, Jr., and L. C. McIntyre, Jr., *Rev. Sci. Instrum.* 50, 1279 (1979).
2. M. D. Burrows, S. R. Ryan, W. E. Lamb, Jr., and L. C. McIntyre, Jr., *J. Chem. Phys.* 71, 4931 (1979).

II. Personnel

We list below personnel associated with this research program:

Principal investigators:

W. E. Lamb, Jr.

B.S. (Chemistry) University of California (Berkeley) 1934

Ph.D. (Physics) University of California (Berkeley) 1938

D.Sc. University of Pennsylvania 1953

M.A. (by decree) Oxford University 1956

M.A. (hon.) Yale University 1961

L.H.D. Yeshiva University 1965

D.Sc. Gustavus Adolphus College 1975

K. C. Hsieh

B.A. (Physics) Wabash College 1963

Ph.D. (Physics) University of Chicago 1969

L. C. McIntyre, Jr.

B.S. (Physics) Stanford University 1957

M.S. (Physics) University of Wisconsin 1961

Ph.D. (Physics) University of Wisconsin 1965

(Professor McIntyre was on sabbatical leave from Aug. 1981 until Aug. 1982. He was replaced as principal investigator by Professor K. C. Hsieh during this period.)

Research Associate:

Otto F. Kalman

B.S. (Chemical Engineering) Purdue University 1955

Ph.D. (Physical Chemistry) Princeton University 1959

Research Assistants:

Richard Cordaro

B.A. Millersville St. College, Penn. 1973

M.S. (Physics) Lehigh University 1978

Bruce Kittams

B.S. Oregon State University 1971

M.S. (Physics) University of Arizona 1981

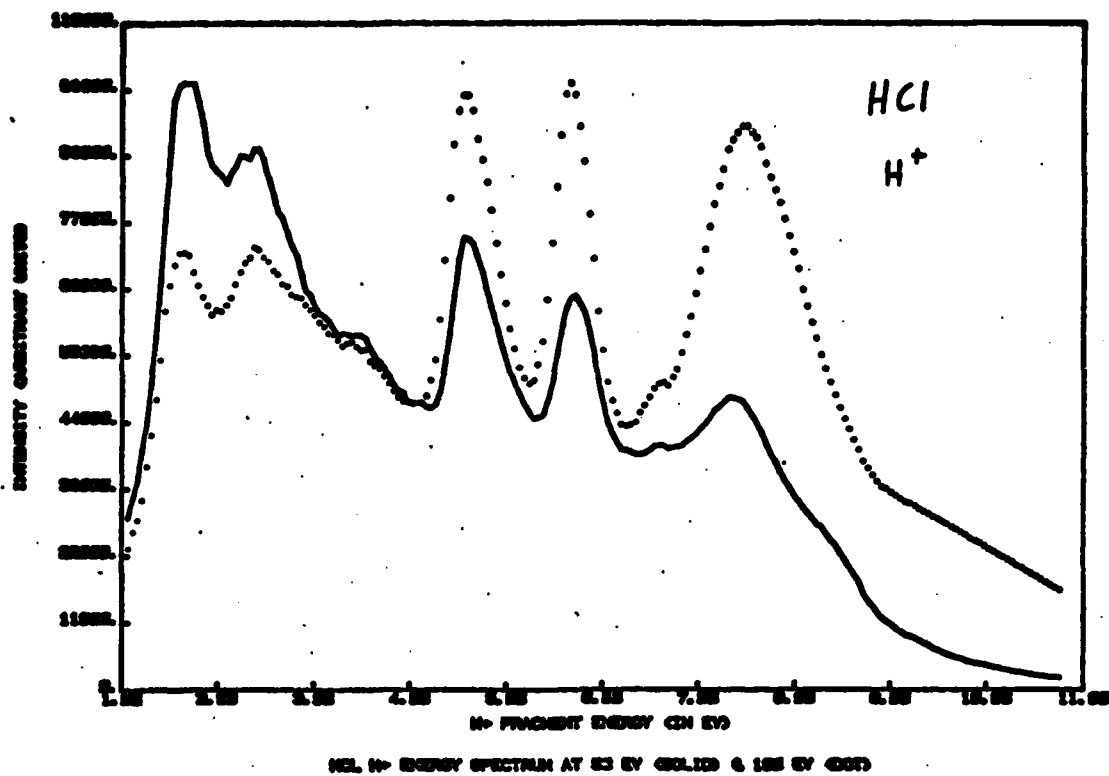


FIGURE 1

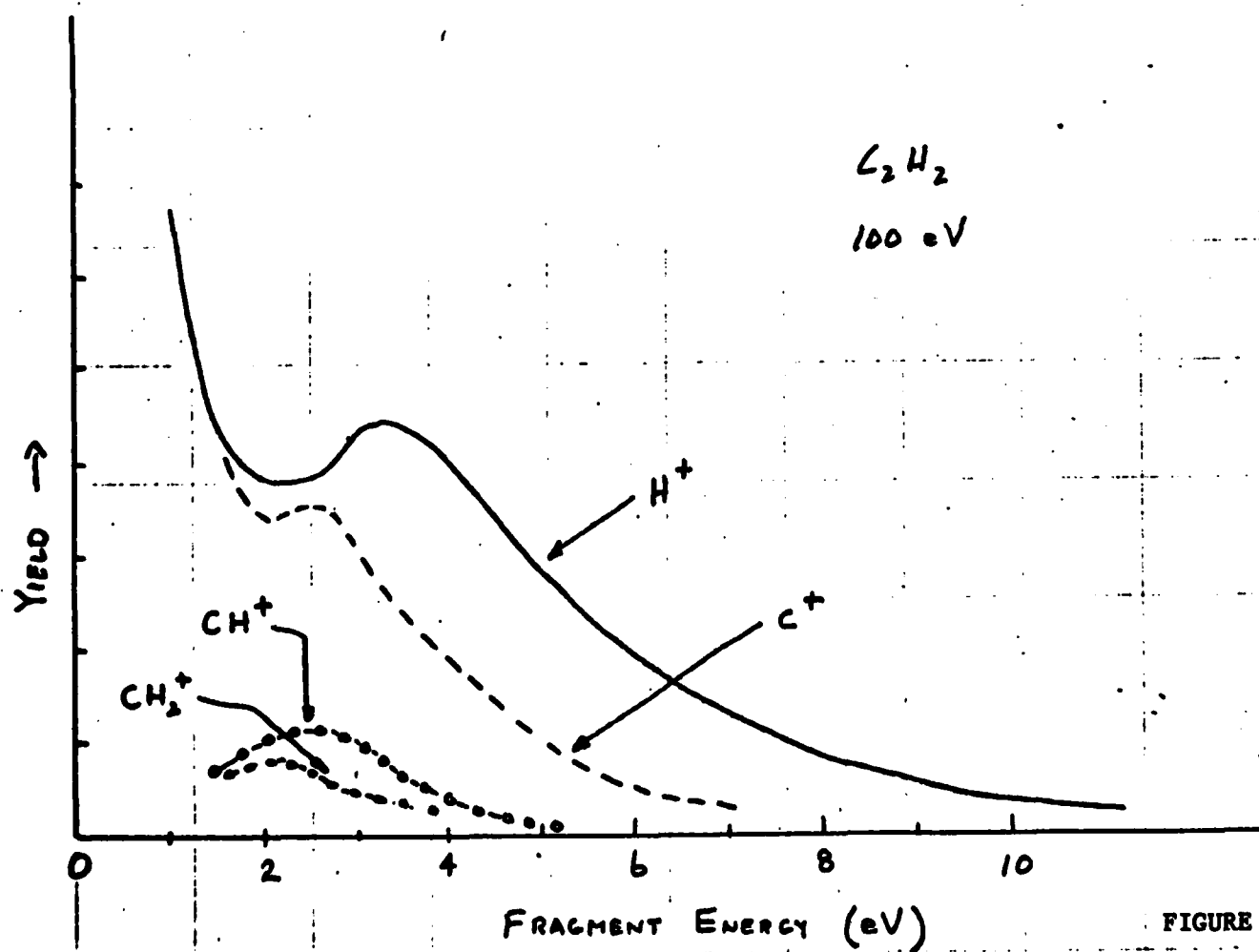


FIGURE 2

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